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L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:909685 CAPLUS
DOCUMENT NUMBER: 134:56837
TITLE: Methods for the production of long-chain substituted estratriene and their application in the preparation of medicaments
INVENTOR(S): Sauer, Gerhard; Bohlmann, Rolf; Heinrich, Nikolaus; Kroll, Jorg; Zorn, Ludwig; Fritzmeier, Karl-Heinrich; Hegele-Hartung, Christa; Hoffmann, Jens; Lichtner, Rosemarie
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19929715	A1	20001228	DE 1999-19929715	19990624
WO 2001000652	A2	20010104	WO 2000-EP5969	20000626
WO 2001000652	A3	20010510		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000061524	A5	20010131	AU 2000-61524	20000626
EP 1187846	A2	20020320	EP 2000-947882	20000626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003503419	T2	20030128	JP 2001-507059	20000626
NO 2001006330	A	20020131	NO 2001-6330	20011221

PRIORITY APPLN. INFO.: DE 1999-19929715 A 19990624
WO 2000-EP5969 W 20000626
OTHER SOURCE(S): MARPAT 134:56837

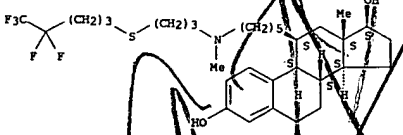
AB This invention describes the synthesis of new antiesterogenic 11.beta. long-chain substituted estratriene [I; R3 = H, alkyl, R3'C(O); R3' = H, alkyl, ph; R11 = ABZR20; A = bond, phenylene, phenyleneoxy; B = alkylene, alkenylene, alkynylene; Z = NR21; R21 = alkyl; R20 = H, alkyl, alkenyl, -alkynyl, DCnFn+1; D = aryl, alkylene, alkenylene, alkynylene; n = 1 - 8; R20 = LCH=CFCpF2p+1; L = alkylene, alkenylene, alkynylene; p = 2-7; R20 = DO(CH2)q-aryl; q = 0 - 3; aryl = Ph, 1-naphthyl, 2-naphthyl, heteroaryl; DO(CH2)rCnF2n+1; r = 1 - 5; R20R21 with N = C5-C6-heterocycle; R20R21 with N = heterocycle etc.; R17 = H, R17'C(O); R17' = H, alkyl] for the prodn. of medicaments. Thus, I [R3, R17 = H; R11 = F5C2(CH2)3S(CH2)3N(Me)(CH2)5] was prepd. from epoxyestrene (II) via reaction with 1-bromo-5-tert-butyldimethylsilyloxypentane, aromatization, chlorination and amination with methyl[3-[(4,4,5,5,5,5-pentafluoropentyl)sulfanyl]propyl]amine. Formulations of I (no data) are claimed.

IT 314019-28-8P 314019-30-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of long-chain substituted estratriene and their application in the prepn. of medicaments)

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

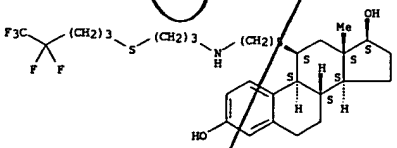
RN 314019-26-6 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



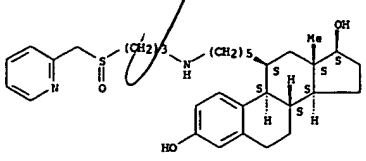
RN 314019-27-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-29-9 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[[3-[(2-pyridinylmethyl)sulfinyl]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

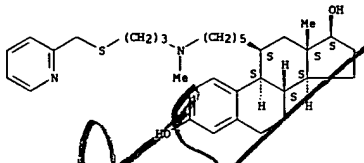
Absolute stereochemistry.



L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

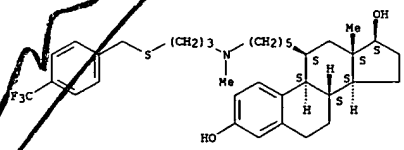
RN 314019-28-8 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[(2-pyridinylmethyl)thio]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 314019-30-2 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[[[4-(trifluoromethyl)phenyl]methyl]thio]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

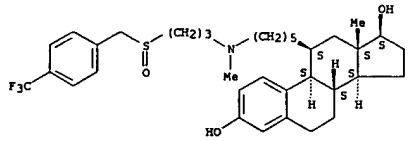


IT 314019-26-6P 314019-27-7P 314019-29-9P
314019-31-3P 314019-58-4P 314019-59-5P
314019-60-8P 314019-61-9P 314019-62-0P
314019-63-1P 314019-65-3P 314019-66-4P
314019-67-5P 314019-68-6P 314019-69-7P
314019-70-0P 314019-71-1P 314019-72-2P
314019-73-3P 314019-74-4P 314019-75-5P
314019-76-6P 314019-77-7P 314019-78-8P
314019-79-9P 314019-80-2P 314019-81-3P
314019-82-4P 314019-83-5P 314019-84-6P
314019-85-7P 314019-86-8P 314019-87-9P
314019-88-0P 314019-89-1P 314019-90-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

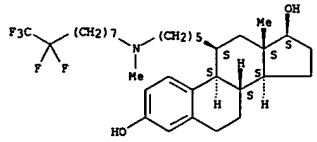
RN 314019-31-3 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[[[4-(trifluoromethyl)phenyl]methyl]sulfinyl]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



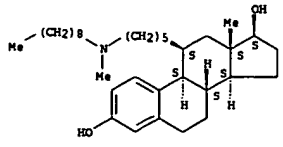
RN 314019-58-4 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(8,8,9,9,9-pentafluorononyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-59-5 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-(methylnonylamino)pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

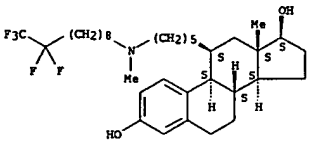
Absolute stereochemistry.



RN 314019-60-8 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(9,9,10,10,10-pentafluorodecyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX

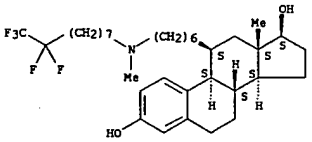
L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
NAME)

Absolute stereochemistry.



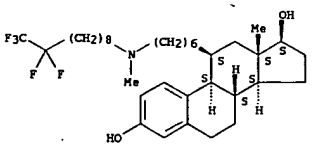
RN 314019-61-9 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[6-[methyl(8,8,9,9,9-pentafluorononyl)amino]hexyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-62-0 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[6-[methyl(9,9,10,10,10-pentafluorodecyl)amino]hexyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

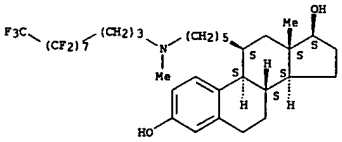
Absolute stereochemistry.



RN 314019-63-1 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-(methylamino)pentyl]-,

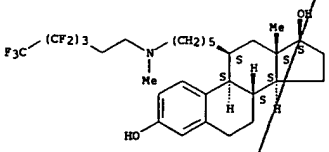
L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
,11,11-heptadecafluoroundecyl)methylamino]pentyl]-, (11.beta.,17.beta.)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



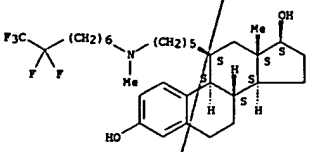
RN 314019-68-6 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(3,3,4,4,5,5,6,6,6-nonafluorohexyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-69-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(7,7,8,8,8-pentafluorooctyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

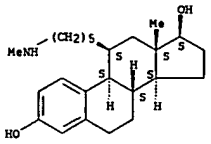
Absolute stereochemistry.



RN 314019-70-0 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[6-[methyl(7,7,8,8,8-pentafluorooctyl)amino]hexyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

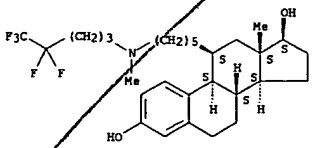
L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



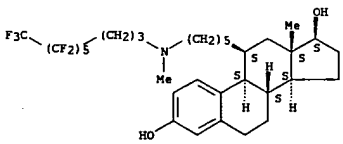
RN 314019-65-3 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(4,4,5,5,5-pentafluoropentyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



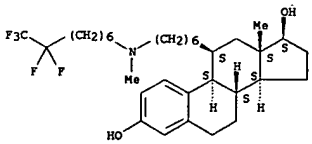
RN 314019-66-4 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluorononyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



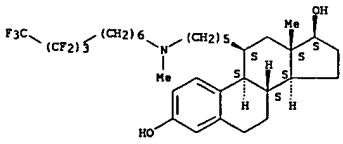
RN 314019-67-5 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(4,4,5,5,6,6,7,7,8,8,9,9,10,10,11

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Absolute stereochemistry.



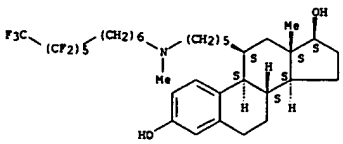
RN 314019-71-1 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(7,7,8,8,9,9,10,10,10-nonafluorodecyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-72-2 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(7,7,8,8,9,9,10,10,11,11,12,12,12-tridecafluorododecyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

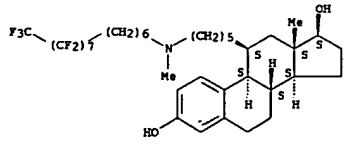
Absolute stereochemistry.



RN 314019-73-3 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-heptadecafluorotetradecyl)methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

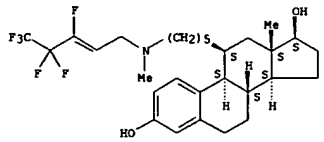
Absolute stereochemistry.

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



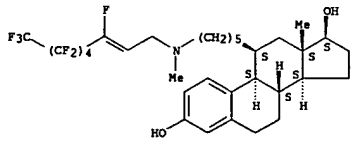
RN 314019-74-4 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(3,4,4,5,5,5-hexafluoro-2-pentenyl)methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 314019-75-5 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(3,4,4,5,5,6,6,7,7,8,8,8-dodecafluoro-2-octenyl)methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

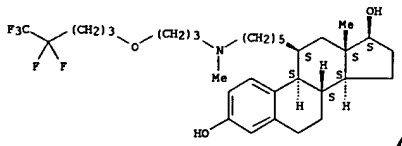
Absolute stereochemistry.
Double bond geometry unknown.



RN 314019-76-6 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-hexadecafluoro-2-decenyl)methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

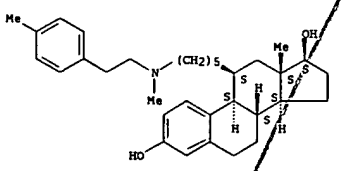
L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(CA INDEX NAME)

Absolute stereochemistry.



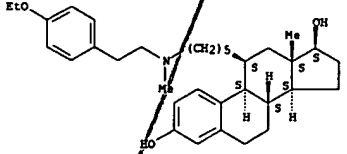
RN 314019-80-2 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[2-(4-methylphenyl)ethyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-81-3 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[[2-(4-ethoxyphenyl)ethyl]methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

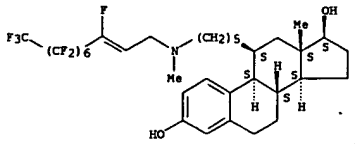
Absolute stereochemistry.



RN 314019-82-4 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(3-phenylpropyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

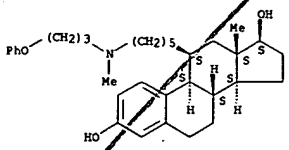
L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.
Double bond geometry unknown.



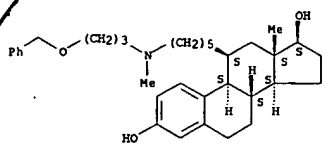
RN 314019-77-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(3-phenoxypropyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



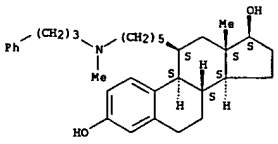
RN 314019-78-8 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-(phenylmethoxy)propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



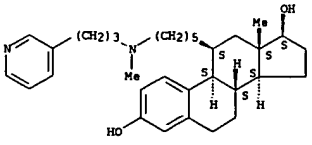
RN 314019-79-9 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)oxy]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI)

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Absolute stereochemistry.



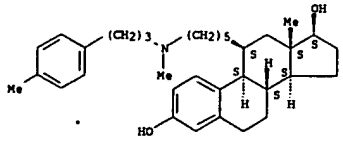
RN 314019-83-5 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-(3-pyridinyl)propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-84-6 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-(4-methylphenyl)propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

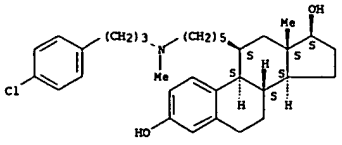
Absolute stereochemistry.



RN 314019-85-7 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[[3-(4-chlorophenyl)propyl]methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

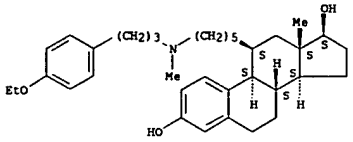
Absolute stereochemistry.

L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



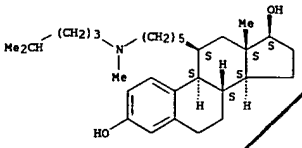
RN 314019-86-8 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[[3-(4-ethoxyphenyl)propyl]methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-87-9 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(4-methylpentyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 314019-88-0 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl(3,4,4,5,5,6,6,6-octafluoro-2-hexenyl)amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

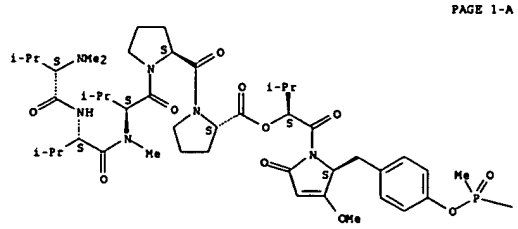
L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:575299 CAPLUS
DOCUMENT NUMBER: 131:170644
TITLE: Preparation of estradiol peptides as antitumor and cytotoxic agents
INVENTOR(S): Jouin, Patrick; Poncet, Joel; Busquet, Magali; Atassi, Ghanem; Pierre, Alain
PATENT ASSIGNEE(S): Adir et Compagnie, Fr.
SOURCE: Fr. Demande, 59 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2774989	A1	19990820	FR 1998-1959	19980218
FR 2774989	B1	20000317		

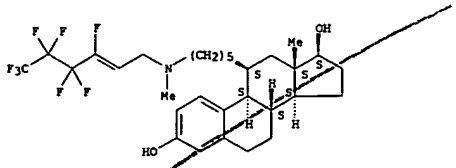
PRIORITY APPLN. INFO.: FR 1998-1959 19980218
OTHER SOURCE(S): MARPAT 131:170644
AB Estradiol peptides E-D-A wherein A represents estradiol I (R1, R2 = independently H, alkyl, alkenyl, arylcarbonyl, arylalkylcarbonyl; R3 = H, bond), D represents acyl, ester, amido, aminoalkylidene, peptide; E represents peptide, dolastatin-15 II (R4 = amidoalkoxy, arylalkylideneamino) were prepd. as antitumor and cytotoxic agents. Thus, peptide III was prepd. and tested in vitro for its antitumor and cytotoxic activities (EC50 = 6.58-1.2 nM).
IT 239117-54-5P 239117-55-6P 239117-56-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of estradiol peptides as antitumor and cytotoxic agents)
RN 239117-54-5 CAPLUS
CN L-Proline, N,N-dimethyl-L-valyl-L-valyl-N-methyl-L-valyl-L-prolyl-, (1S)-1-[[(2S)-2-[[4-[[[4-[[2-[(11.beta.,17.beta.)-3,17-dihydroxyestra-1,3,5(10)-trien-11-yl]ethyl]amino]-4-oxobutoxy]methylphosphinyl]oxy]phenyl]methyl]-2,5-dihydro-3-methoxy-5-oxo-1H-pyrrol-1-yl]carbonyl]-2-methylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

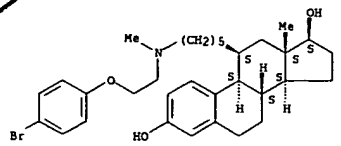


L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



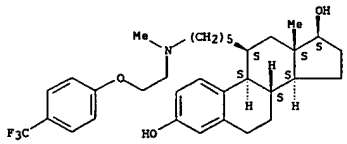
RN 314019-89-1 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[[2-(4-bromophenoxy)ethyl]methylamino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



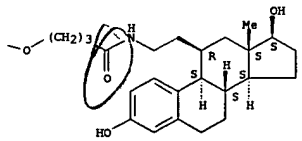
RN 314019-90-4 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[2-[4-(trifluoromethyl)phenoxy]ethyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

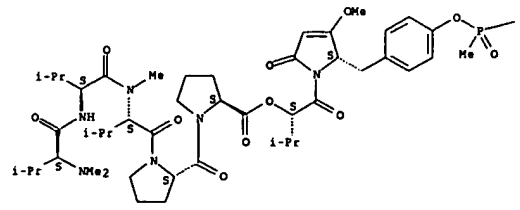
PAGE 1-B



RN 239117-55-6 CAPLUS
CN L-Proline, N,N-dimethyl-L-valyl-L-valyl-N-methyl-L-valyl-L-prolyl-, (1S)-1-[[(2S)-2-[[4-[[[4-[[4-[(11.beta.,17.beta.)-3,17-dihydroxyestra-1,3,5(10)-trien-11-yl]butyl]amino]-4-oxobutoxy]methylphosphinyl]oxy]phenyl]methyl]-2,5-dihydro-3-methoxy-5-oxo-1H-pyrrol-1-yl]carbonyl]-2-methylpropyl ester (9CI) (CA INDEX NAME)

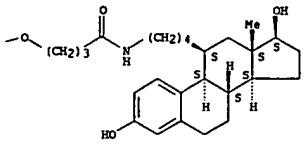
Absolute stereochemistry.

PAGE 1-A



L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

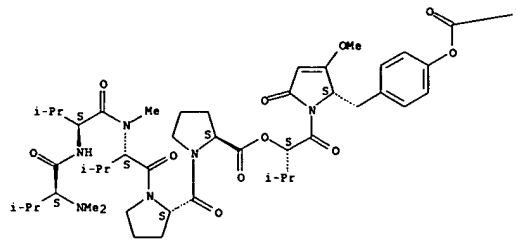
PAGE 1-B



RN 239117-56-7 CAPLUS
CN L-Proline, N,N-dimethyl-L-valyl-L-valyl-N-methyl-L-valyl-L-prolyl-, (1S)-1-[[(2S)-2-[[4-[[6-[[2-[(11.beta.,17.beta.)-3,17-dihydroxyestra-1,3,5(10)-trien-11-yl]ethyl]amino]-1,6-dioxohexyl]oxy]phenyl]methyl]-2,5-dihydro-3-methoxy-5-oxo-1H-pyrrol-1-yl]carbonyl]-2-methylpropyl ester (9CI) (CA INDEX NAME)

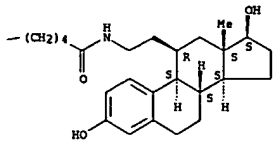
Absolute stereochemistry.

PAGE 1-A



L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-B



L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

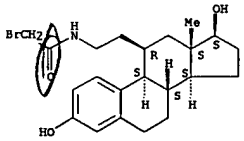
ACCESSION NUMBER: 1997:435821 CAPLUS
DOCUMENT NUMBER: 127:76140
TITLE: Steroidal Affinity Labels of the Estrogen Receptor. 3. Estradiol 11.beta.-n-Alkyl Derivatives Bearing a Terminal Electrophilic Group: Antiestrogenic and Cytotoxic Properties
AUTHOR(S): Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; Nique, Francois; Teutsch, Georges; Borgna, Jean-Louis
CORPORATE SOURCE: INSERM Unite 439, Montpellier, 34090, Fr.
SOURCE: Journal of Medicinal Chemistry (1997), 40(14), 2217-2227
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB With the aim of developing a new series of steroidal affinity labels of the estrogen receptor, six electrophilic 11.beta.-Et (C2), 11.beta.-Bu (C4), or 11.beta.-decyl (C10) derivs. of estradiol bearing 11.beta.-terminal electrophilic functionalities, i.e. bromine (C4), (methylsulfonyl)oxy (C2 and C4), bromoacetamido (C2 and C4), and (p-tolylsulfonyl)oxy (C10) were synthesized. The range of their affinity consts. for binding the estrogen receptor was 0.4-37% that of estradiol; the order of increasing affinity (i) relative to the 11.beta.-alkyl arm was Et < Bu and (ii) relative to the electrophilic functionalities was bromoacetamido < bromine < (methylsulfonyl)oxy. Regardless of the conditions used, including prolonged exposure of the receptor to various pH levels (7-9) and temps. (0-25.degree.), the extent of receptor affinity labeling by the 11.beta.-Et and 11.beta.-Bu compds., if any, was under 10%. This was in sharp contrast to results obtained using 11.beta.-[(tosyloxy)decyl]estradiol which labeled from 60% to 90% of the receptor hormone-binding sites with an EC50 of .apprx.10 nM. Estrogenic and antiestrogenic activities of the compds. were detd. using the MVLN cell line, which was established from the estrogen-responsive mammary tumor MCF-7 cells by stable transfection of a recombinant estrogen-responsive luciferase gene. The two 11.beta.-Et compds. were mainly estrogenic, whereas the three 11.beta.-Bu and the 11.beta.-decyl compds. essentially showed antiestrogenic activity. The fact that the chem. reactivities of 11.beta.-Et and 11.beta.-Bu compds. were not compromised by interaction with the estrogen receptor made the synthesized high-affinity compds. potential cytotoxic agents which might be able to exert either (i) a specific action on estrogen-regulated genes or (ii) a more general action in estrogen-target cells. Therefore the ability of the compds. (1) to irreversibly abolish estrogen-dependent expression of the luciferase gene and (2) to affect the proliferation of MVLN cells was detd. All electrophiles were able to irreversibly suppress expression of the luciferase gene; the antiestrogenic electrophiles were more potent than the estrogenic ones but less efficient than 4-hydroxytamoxifen, a classical and chem. inert triphenylethylene antiestrogen. Only the antiestrogenic electrophiles decreased cell proliferation; however, they were less potent than 4-hydroxytamoxifen. In conclusion, the synthesized electrophilic estradiol 11.beta.-Et and 11.beta.-Bu derivs. (i) were not efficient affinity labels of the estrogen receptor and (ii) did not display significant cytotoxicity in estrogen-sensitive mammary tumor cells. However, since these derivs. displayed high affinity for the estrogen receptor, they could be used to prep. potential cytotoxic agents which might be selective for tumors affecting estrogen-target tissues, by coupling them with a toxic moiety.

IT 191486-88-1P 191487-03-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of estradiol 11.beta.-n-alkyl derivs. as steroidal affinity labels of the estrogen receptor)

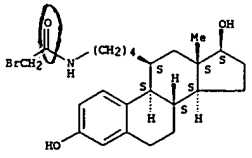
RN 191486-88-1 CAPLUS
CN Acetamide, 2-bromo-N-[2-[(11.beta.,17.beta.)-3,17-dihydroxyestra-1,3,5(10)-trien-11-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 191487-03-3 CAPLUS
CN Acetamide, 2-bromo-N-[4-[(11.beta.,17.beta.)-3,17-dihydroxyestra-1,3,5(10)-trien-11-yl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

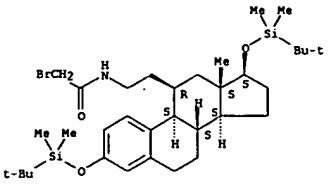


IT 191486-87-0P 191487-02-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of estradiol 11.beta.-n-alkyl derivs. as steroidal affinity labels of the estrogen receptor)

RN 191486-87-0 CAPLUS
CN Acetamide, N-[2-[(11.beta.,17.beta.)-3,17-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]estra-1,3,5(10)-trien-11-yl]ethyl]-2-bromo- (9CI) (CA INDEX NAME)

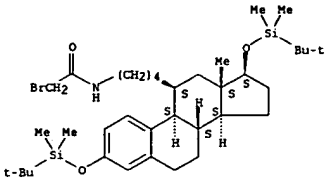
Absolute stereochemistry.

L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 191487-02-2 CAPLUS
CN Acetamide, N-[4-[(11.beta.,17.beta.)-3,17-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]estra-1,3,5(10)-trien-11-yl]butyl]-2-bromo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:656464 CAPLUS
DOCUMENT NUMBER: 115:256464
TITLE: Preparation of 19-norsteroids containing an amide or a carboxamide group as drugs
INVENTOR(S): Claussner, Andre; Nedelec, Lucien; Philibert, Daniel; Van de Velde, Patrick
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: Eur. Pat. Appl., 128 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 384842	A1	19900829	EP 1990-400493	19900222
EP 384842	B1	19931229		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL				
FR 2643638	A1	19900831	FR 1989-2384	19890224
FR 2643638	B1	19910614		
HU 55032	A2	19910429	HU 1990-273	19900125
HU 207341	B	19930329		
ZA 9001356	A	19910424	ZA 1990-1356	19900222
AT 99320	E	19940115	AT 1990-400493	19900222
ES 2062431	T3	19941216	ES 1990-400493	19900222
CA 2010826	AA	19900824	CA 1990-2010826	19900223
AU 9050072	A1	19900830	AU 1990-50072	19900223
AU 631853	B2	19921210		
JP 02268194	A2	19901101	JP 1990-41383	19900223
JP 3009169	B2	20000214		
US 5149696	A	19920922	US 1990-484424	19900223
PL 162151	B1	19930930	PL 1990-283941	19900223
CN 1046166	A	19901017	CN 1990-101580	19900224
US 5290771	A	19940301	US 1992-875460	19920429
US 5707982	A	19980113	US 1993-68735	19930528

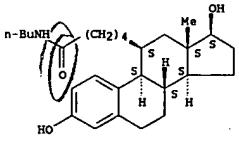
PRIORITY APPLN. INFO.: FR 1989-2384 A 19890224
EP 1990-400493 A 19900222
US 1990-484424 A3 19900223
FR 1990-10323 A 19900814
US 1991-745289 B1 19910814

OTHER SOURCE(S): CASREACT 115:256464; MARPAT 115:256464

AB The title compds. [I; R, R1 = H, (substituted) alkyl; or NRR1 = (substituted) heterocyclyl; R2 = OH, acyloxy; R3 = H, (substituted) alkyl, alkenyl, alkynyl; or R2R3 = O; X = CH2, arylene, CH2O, aryleneoxy linked to the steroid moiety by C; Y = bond, (substituted) aliph. chain; Z = bond, CH2O linked to Y by C; rings A and B may be (2-substituted) Q, Q1; R4 = H, alkyl], having affinities for receptors of hormones, e.g., estrogen, androgen, progesterone, and therefore useful as inhibitors of hormone-dependent tumors and many other ailments, were prepd. Estradienone II [R5 = OH] [prepd. in several steps from epoxyestrenedione III and p-Me3CSiMe2O(CH2)8C6H4Br] was amidated with HNMeBu to give II (R5 = NMeBu), which was enol-esterified with AcBr and the product hydrolyzed to give I [R = Me, R1 = Bu, X = C6H4, Y = (CH2)7, Z = bond, R2 = OH, rings A and B = Q1, R3 = R4 = H]. This had an IC50 of 0.04 .mu.M against the growth of mammary tumor cells.

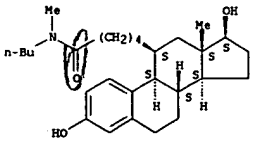
L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
IT **134411-65-7P 134411-66-8P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as drug)
RN 134411-65-7 CAPLUS
CN Estra-1,3,5(10)-triene-11-pentanamide, N-butyl-3,17-dihydroxy-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 134411-66-8 CAPLUS
CN Estra-1,3,5(10)-triene-11-pentanamide, N-butyl-3,17-dihydroxy-N-methyl-, (11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

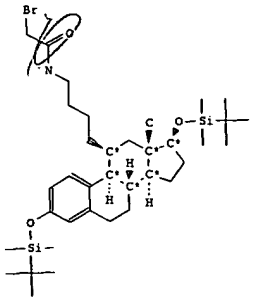
Absolute stereochemistry.



=> d all 1-4

L9 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	7842637
Chemical Name (CN):	N-<4-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-butyl>-2-bromo-acetamide
Autonom Name (AUN):	N-<4-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-butyl>-2-bromo-acetamide
Molec. Formula (MF):	C36 H62 Br N O3 Si2
Molecular Weight (MW):	692.97
Lawson Number (LN):	15224, 3798, 3777, 1155
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	6729739
Tautomer ID (TAUTID):	7453813
Beilstein Citation (BSO):	6-13
Entry Date (DED):	1998/04/30
Update Date (DUPD):	1998/05/04



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1

L9 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

Reaction:
RX

Reaction ID (.ID):	4781161
Reactant BRN (.RBRN):	7838449, 506167
Reactant (.RCT):	4-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-butylamine, bromoacetic acid
Product BRN (.PBRN):	7842637
Product (.PRO):	N-<4-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-butyl>-2-bromo-acetamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	4781161.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	1-ethyl-3-<3-(dimethylamino)propyl>carbodiimide hydrochloride, pyridine
Solvent (.SOL):	tetrahydrofuran
Time (.TIM):	30 min
Temperature (.T):	40 Cel
Reference(s):	

1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Reaction:
RX

Reaction ID (.ID):	4804487

L9 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

Reactant BRN (.RBRN):	7842637
Reactant (.RCT):	N-<4-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-butyl>-2-bromo-acetamide
Product BRN (.PBRN):	7833530
Product (.PRO):	2-bromo-N-<4-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl)-butyl>-acetamide
No. of React. Details (.NVAR):	1

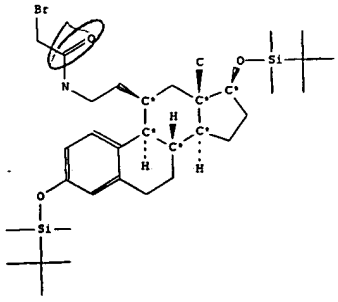
Reaction Details:
RX

Reaction RID (.RID):	4804487.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	aq. AcOH
Solvent (.SOL):	tetrahydrofuran
Time (.TIM):	20 hour(s)
Other Conditions (.COND):	Ambient temperature
Note(s) (.COM):	Yield given
Reference(s):	

1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

L9 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	7840634
Chemical Name (CN):	N-<2-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-ethyl>-2-bromo-acetamide
Autonom Name (AUN):	N-<2-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-ethyl>-2-bromo-acetamide
Molec. Formula (MF):	C34 H58 Br N O3 Si2
Molecular Weight (MW):	664.91
Lawson Number (LN):	15230, 3798, 3777, 1155
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	6727235
Tautomer ID (TAUTID):	7451996
Beilstein Citation (BSO):	6-13
Entry Date (DED):	1998/04/30
Update Date (DUPD):	1998/05/04



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1

L9 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

LN	Lawson Number	4
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

Reaction:
RX

Reaction ID (.ID):	4781159
Reactant BRN (.RBRN):	7836551, 506167
Reactant (.RCT):	2-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-ethylamine, bromoacetic acid
Product BRN (.PBRN):	7840634
Product (.PRO):	N-<2-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-ethyl>-2-bromo-acetamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	4781159.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	1-ethyl-3-<3-(dimethylamino)propyl>carbodiimide hydrochloride, pyridine
Solvent (.SOL):	tetrahydrofuran
Time (.TIM):	30 min
Temperature (.T):	40 Cel
Reference(s):	

1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Reaction:
RX

Reaction ID (.ID):	4803841
Reactant BRN (.RBRN):	7840634
Reactant (.RCT):	N-<2-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-ethyl>-2-bromo-acetamide
Product BRN (.PBRN):	7829440
Product (.PRO):	2-bromo-N-<2-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl)-ethyl>-acetamide
No. of React. Details (.NVAR):	1

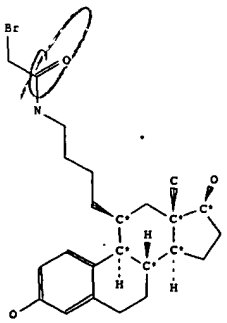
Reaction Details:
RX

Reaction RID (.RID):	4803841.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	aq. AcOH
Solvent (.SOL):	tetrahydrofuran
Time (.TIM):	20 hour(s)
Other Conditions (.COND):	Ambient temperature
Note(s) (.COM):	Yield given
Reference(s):	

1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

L9 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	7833530
Chemical Name (CN):	2-bromo-N-<4-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl)-butyl>-acetamide
Autonom Name (AUN):	2-bromo-N-<4-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl)-butyl>-acetamide
Molec. Formula (MF):	C24 H34 Br N O3
Molecular Weight (MW):	464.44
Lawson Number (LN):	15224, 1155
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	6717041
Tautomer ID (TAUTID):	7450857
Beilstein Citation (BSO):	6-13
Entry Date (DED):	1998/04/30
Update Date (DUPD):	1998/05/04



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
MW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1

L9 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value (MP) (Cel)	Solvent (.SOL)	Ref.	Note
240	diethyl ether	1	1

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Notes(s):
1. 50

Nuclear Magnetic Resonance:
NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	1H
Solvents (.SOL):	dimethylsulfoxide-d6
Temperature (.T):	32 Cel
Reference(s):	

1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

NMR

Description (.KW):	Spin-spin coupling constants
Solvents (.SOL):	dimethylsulfoxide-d6
Temperature (.T):	32 Cel
Note(s) (.COM):	1H-1H.
Reference(s):	

1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Infrared Spectrum:

L9 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Description (.KW)	Solvent (.SOL)	Ref.	Note
Bands	KBr	1	1

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Notes(s):
1. 3535 - 1675 cm**(-1)

Pharmacological Data:
PHARM

Note(s) (.COM):	binding affinity to the estrogen receptor; estrogen antagonist activity, IC50: 320 nM (MVLN cell line); antiproliferative activity (ability to promote DNA accumulation from MVLN)

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Reaction:
RX

Reaction ID (.ID):	4804487
Reactant BRN (.RBRN):	7842637
Reactant (.RCT):	N-<4-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-butyl>-2-bromo-acetamide
Product BRN (.PBRN):	7833530
Product (.PRO):	2-bromo-N-<4-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl)-butyl>-acetamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

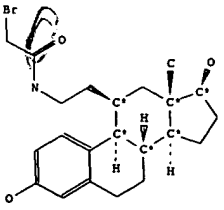
Reaction RID (.RID):	4804487.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	aq. AcOH
Solvent (.SOL):	tetrahydrofuran
Time (.TIM):	20 hour(s)
Other Conditions (.COND):	Ambient temperature
Note(s) (.COM):	Yield given

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14),

L9 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)
<1997>, 2217-2227; BABS-6075367

L9 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	7829440
Chemical Name (CN):	2-bromo-N-<2-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl)-ethyl>-acetamide
Autonom Name (AUN):	2-bromo-N-<2-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl)-ethyl>-acetamide
Molec. Formula (MF):	C22 H30 Br N O3
Molecular Weight (MW):	436.39
Lawson Number (LN):	15230, 1155
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	6711546
Tautomer ID (TAUTID):	7447711
Beilstein Citation (BSO):	6-13
Entry Date (DED):	1998/04/30
Update Date (DUPD):	1998/05/04



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
MW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1

L9 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Melting Point:

Value (MP) (Cel)	Solvent (.SOL)	Ref.
170 - 172	diethyl ether	1

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Nuclear Magnetic Resonance:
NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	1H
Solvents (.SOL):	CDCl3
Temperature (.T):	32 Cel

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

NMR

Description (.KW):	Spin-spin coupling constants
Solvents (.SOL):	CDCl3
Temperature (.T):	32 Cel
Note(s) (.COM):	1H-1H.

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Infrared Spectrum:

Description (.KW)	Solvent (.SOL)	Ref.	Note
Bands	KBr	1	1

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

L9 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Notes(s):
1. 3520 - 1685 cm**(-1)

Pharmacological Data:
PHARM

Note(s) (.COM):	binding affinity to the estrogen receptor; estrogen agonist activity, EC50: 110 nM (MVLN cell line); proliferative activity (ability to promote DNA accumulation from MVLN)

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

Reaction:
RX

Reaction ID (.ID):	4803841
Reactant BRN (.RBRN):	7840634
Reactant (.RCT):	N-<2-<3,17-bis-(tert-butyl-dimethyl-silanyloxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl>-ethyl>-2-bromo-acetamide
Product BRN (.PBRN):	7829440
Product (.PRO):	2-bromo-N-<2-(3,17-dihydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-11-yl)-ethyl>-acetamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	4803841.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	aq. AcOH
Solvent (.SOL):	tetrahydrofuran
Time (.TIM):	20 hour(s)
Other Conditions (.COND):	Ambient temperature
Note(s) (.COM):	Yield given

Reference(s):
1. Lobaccaro, Carole; Pons, Jean-Francois; Duchesne, Marie-Josephe; Auzou, Gilles; Pons, Michel; et al., J.Med.Chem., CODEN: JMCMAR, 40(14), <1997>, 2217-2227; BABS-6075367

=> d ibib ab fqhit 1-7

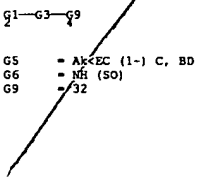
L11 ANSWER 1 OF 7 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 135:16357 MARPAT
TITLE: Steroid compounds for steroid receptor binding assays
INVENTOR(S): Schoonen, Wilhelmus G. E. J.
PATENT ASSIGNEE(S): Akzo Nobel N.V., Neth.
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001040805	A1	20010607	WO 2000-EP11803	20001124
W: US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1238285	A1	20020911	EP 2000-989893	20001124
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.: EP 1999-204036 19991130
WO 2000-EP11803 20001124

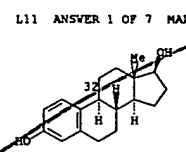
AB The invention provides a compd. having binding affinity for a receptor and comprising a steroid skeleton in its mol. structure, which compd. is Bu-A-Y-X-Ste (Bu = sterically bulky structure or mol. moiety having high affinity for a sterically bulky mol. structure; A = -NH-, -O-, -C(O)-, -S-; Y = branched or unbranched, satd. or unsatd. chain of 2 to 18 atoms of carbon, which chain is optionally interrupted by replacements of carbon atoms by oxygen, nitrogen or sulfur atoms and is optionally substituted with keto, hydroxyl, sulfhydryl or halogen groups; X = C or arylene group linked to the steroid skeleton with a carbon or an oxygen atom; Ste = group with a steroidal skeleton, having binding affinity for a steroid receptor; the bond between A and Y is optional double or triple bond; that between Y and X is optional double bond). The invention also provides for a method for detn. of binding between a compd. having a mol. group L in its mol. structure and a compd. having a mol. group R in its mol. structure, in which method L is the group Ste as defined above and R is a steroid receptor. An estradiol estrogen receptor ligand labeled with allophycocyanin (steroid-APC) was prepd. and assayed for binding with the .alpha.-estrogen receptor by time-resolved fluorescence resonance energy transfer assay.

MSTR 1



G5 = Ak<EC (1-) C, BD (0-) D (0-) T> (SO)
G6 = NH (SO)
G9 = 32

L11 ANSWER 1 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



MPL: claim 1
NTE: or addition salts or solvates
NTE: also incorporates claim 12

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 7 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 134:56837 MARPAT
TITLE: Methods for the production of long-chain substituted estratriene and their application in the preparation of medicaments
INVENTOR(S): Sauer, Gerhard; Bohlmann, Rolf; Heinrich, Nikolaus; Kroll, Jorg; Zorn, Ludwig; Fritzmeier, Karl-Heinrich; Hegele-Hartung, Christa; Hoffmann, Jens; Lichtner, Rosemarie
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

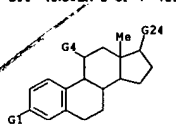
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19929715	A1	20001228	DE 1999-19929715	19990624
WO 2001000652	A2	20010104	WO 2000-EP5969	20000626
WO 2001000652	A3	20010510		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000061524	A5	20010131	AU 2000-61524	20000626
EP 1187846	A2	20020320	EP 2000-947882	20000626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003503419	T2	20030128	JP 2001-507059	20000626
NO 2001006330	A	20020131	NO 2001-6330	20011221

PRIORITY APPLN. INFO.: DE 1999-19929715 19990624
WO 2000-EP5969 20000626

AB This invention describes the synthesis of new antiesterogenic 11.beta. long-chain substituted estratriene [I; R3 = H, alkyl, R3'C(O); R3' = H, alkyl, ph; R11 = ABZR20; A = bond, phenylene, phenyleneoxy; B = alkylene, alkenylene, alkynylene; Z = NR21; R21 = alkyl; R20 = H, alkyl, alkenyl, -alkynyl, DCnFn+1; D = aryl, alkylene, alkenylene, alkynylene; n = 1 - 8; R20 = LCH=CFCpF2p+1; L = alkylene, alkenylene, alkynylene; p = 2-7; R20 = DO(CH2)q-aryl; q = 0 - 3; aryl = Ph, 1-naphthyl, 2-naphthyl, heteroaryl; DO(CH2)rCnF2n+1; r = 1 - 5; R20R21 with N = C5-C6-heterocycle; R20R21 with N = heterocycle etc.; R17 = H, R17'C(O); R17' = H, alkyl] for the prodn. of medicaments. Thus, I [R3, R17 = H; R11 = F5C2(CH2)3S(CH2)3N(Me)(CH2)5] was prepd. from 3-oxyestrene (II) via reaction with 1-bromo-5-tert-butyldimethylsilyloxypentane, aromatization, chlorination and amination with methyl(3-[(4,4,5,5,5,5-pentafluoropentyl)sulfanyl]propyl)amine. Formulations of I (no data) are claimed.

MSTR 1

L11 ANSWER 2 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G1 = OH
G5 = alkylene<(4-6)>
G9 = alkylamino<(1-3)>
G24 = OH
MPL: claim 1

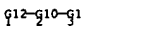
L11 ANSWER 3 OF 7 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 131:170644 MARPAT
TITLE: Preparation of estradiol peptides as antitumor and cytotoxic agents
INVENTOR(S): Jouin, Patrick; Poncet, Joel; Busquet, Magali; Atassi, Ghanem; Pierre, Alain
PATENT ASSIGNEE(S): Adir et Compagnie, Fr.
SOURCE: Fr. Demande, 59 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2774989	A1	19990820	FR.1998-1959	19980218
FR 2774989	B1	20000317		

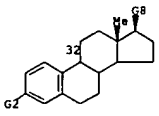
PRIORITY APPLN. INFO.: FR 1998-1959 19980218

AB Estradiol peptides E-D-A wherein A represents estradiol I (R1, R2 = independently H, alkyl, alkenyl, acylcarbonyl, arylalkylcarbonyl; R3 = H, bond), D represents acyl, ester, amido, aminoalkylidene, peptide; E represents peptide, dolastatin-15 II (R4 = amidoalkoxy, arylalkylideneamino) were prepd. as antitumor and cytotoxic agents. Thus, peptide III was prepd. and tested in vitro for its antitumor and cytotoxic activities (EC50 = 6.58-1.2 nM).

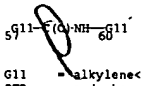
MSTR 1



G1 = 32



G2 = OH
G8 = OH
G10 = 57-1 60-3



G11 = alkylene<(1-6)>
DER: and pharmaceutically acceptable acid or base addition salts
MPL: claim 1

L11 ANSWER 3 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)
STE: and isomers

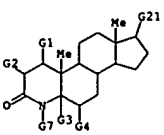
L11 ANSWER 4 OF 7 MARPAT COPYRIGHT 2003 ACS on STN
(ALL HITs ARE ITERATION INCOMPLETES)
ACCESSION NUMBER: 121:109397 MARPAT
TITLE: Preparation of ester derivatives of 4-azasteroids as steroid 5.alpha.-reductase inhibitors.
INVENTOR(S): Witzel, Bruce E.; Rasmusson, Gary H.; Tolman, Richard L.; Yang, Shu Shu
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9323041	A1	19931125	WO 1993-US4771	19930519
W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9342525	A1	19931213	AU 1993-42525	19930519
AU 668181	B2	19960426		
EP 649306	A1	19950426	EP 1993-911362	19930519
EP 649306	B1	20010110		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07508039	T2	19950907	JP 1993-503838	19930519
AT 198601	E	20010115	AT 1993-911362	19930519
US 5610162	A	19970311	US 1994-338573	19941117

PRIORITY APPLN. INFO.: US 1992-886022 19920520
WO 1993-US4771 19930519

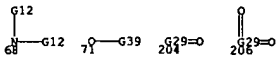
AB Title compds. [I; a, b = single bonds, R2 = H; or a = single bond, b = double bond, and R2 = null; R1 = H, aryl, alkyl, aralkyl; R3 = H, Me, Et, OH, NH2, SMe; n = 0-10; X = O, S; R4 = (substituted) alkyl, aryl, heterocyclyl, cycloalkyl, amino, OH, etc.] were prepd. as inhibitors of 5.alpha.-reductase and isoenzymes thereof. The compds. are useful for the treatment of hyperandrogenic disease conditions and diseases of the skin and scalp (no data). Thus, 20-hydroxy-4-methyl-5.alpha.-4-azapregnan-3-one, 11-ethylthioundecanoic acid, DMAP, and DCC were stirred in CH2Cl2 at room temp. to give 20-[11-(ethylthio)undecanoyloxy]-4-methyl-5.alpha.-4-azapregnan-3-one.

MSTR 1 ITERATION INCOMPLETE

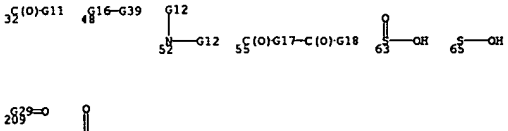


G1 = H
G2 = H
G3 = H
G4 = H

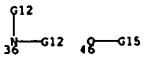
L11 ANSWER 4 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)
G5 = NULL / G40 / alkylene<EC (1-10) C, DC (0) M3> (SO (1-) G6)
G6 = Ph / naphthyl / alkyl<(1-3)> (SO G28) / (SC Me)
G7 = H / Me / Et / OH / NH2 / SMe
G8 = O / S
G9 = Ph (SO) / naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> (SO) / 204 / 206 / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO) / cycloalkyl<(3-10)> (SO) / 68 / OH / 71



G10 = OH / F / Cl / Br / I / alkoxy<(1-8)> / alkenyl<(2-6)> / 32 / SH / 65 / 63 / 48 / 52 / Ph (SO) / naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> (SO) / 209 / 211 / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO) / cycloalkyl<(3-10)> (SO) / 55

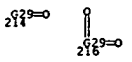


G11 = 36 / OH / 46

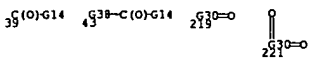


G12 = H / alkyl<(1-8)> (SO (1-) G13) / Ph (SO) / naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> (SO) / 214 / 216 / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO)

L11 ANSWER 4 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G13 = OH / alkoxy<(1-3)> / CN / 39 / 43 / NO2 / F / Cl / Br / I / NH2 / alkylamino<(1-4)> / dialkylamino<(1-4)> / Ph (SO) / naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> / 219 / 221 / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER>



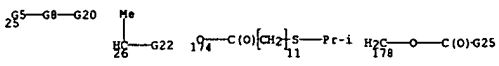
G14 = OH / 41

G15 = alkyl<(1-8)> (SO) / Ph (SO) / naphthyl (SO)
G16 = S / S(O) / SO2
G17 = NH / 59

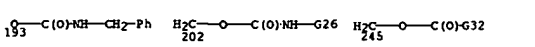
G18 = NH2 / 61

G19 = alkyl<(1-8)> / CH2Ph / cyclohexyl
G20 = alkylcarbonyl<(1-20)> (SO (1-) G10) / 30

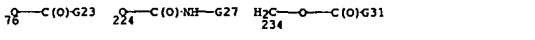
G21 = 25 / (SC 26 / 174 / 178 / 193 / 202) / (EX 245 / 330)

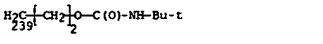


L11 ANSWER 4 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

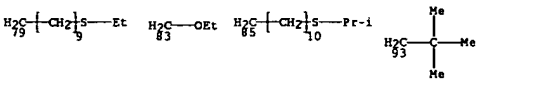


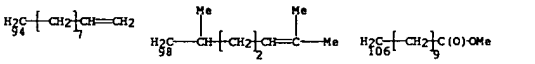
G22 = 76 / 224 / 234 / 239

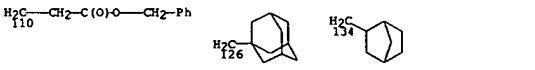


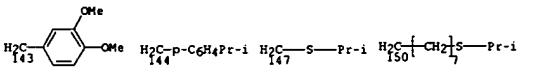


G23 = 79 / 83 / 85 / dodecyl / 93 / Bu-t / 94 / 98 / CH2CH2CO2H / 106 / 110 / 126 / 134 / 143 / 144 / 147 / 150 / 154 / 158 / 169

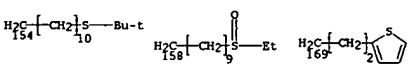




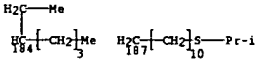




L11 ANSWER 4 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



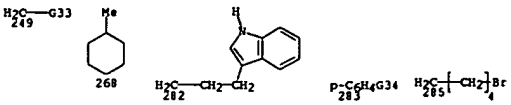
G25 = Me / Bu-t / 184 / 187



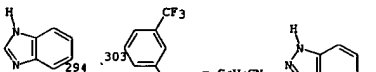
G26 = Bu-t / Me / 228

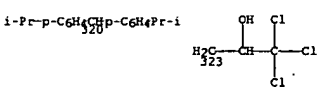
G27 = Bu-t / Pr-i / Me
G28 = Ph / naphthyl
G29 = Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO)
G30 = Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER>
G31 = Me / Bu-t / 235

G32 = 249 / 268 / 282 / 283 / 285 / 294 / 303 / 306 / 314 / 320 / 323 / CH=CHPh

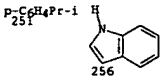


L11 ANSWER 4 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

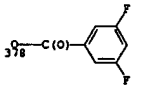




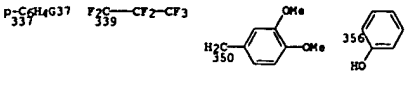
G33 = 2-furyl / 251 / cyclohexyl / 256 / OCOMe



G34 = Bu-i / OEt
G35 = 333 / 358 / 373 / 378

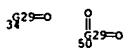


G36 = 337 / pentadecyl / 339 / 350 / 356



G37 = NO2 / COPh
G38 = alkylene<(1-8)>
G39 = alkyl<(1-8)> (SO (1-) G13) / Ph (SO) / naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> (SO) / 34 / 50 / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO)

L11 ANSWER 4 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



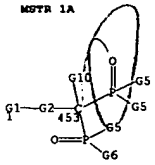
G40 = (1-10) CH2
G1 +G2 = NULL
G3 +G4 = NULL
DER: or pharmaceutically acceptable salts or ester
MPL: claim 1
NTE: up to one double bond in steroid moiety

L11 ANSWER 5 OF 7 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 120:134926 MARPAT
TITLE: Preparation of estrogen bisphosphonates for treatment of bone diseases
INVENTOR(S): Nakamura, Toshio; Katsumata, Takashi; Yamamoto, Michihiro
PATENT ASSIGNEE(S): Sumitomo Pharma, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 33 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

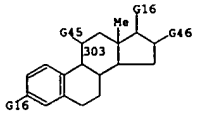
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05222073	A2	19930831	JP 1992-59642	19920213
PRIORITY APPLN. INFO.:			JP 1992-59642	19920213

AB The title compds. [I; E = estrogen residue; R1 = bond, alkylene; R2 = alkylene, alkenylene, alkynylene; R3 = H, alkyl; R4 = OH, alkyl, alkoxy; Y1 = bond, O, S(O)n (wherein n = 0, 1, 2), NR5 (wherein R5 = H, alkyl), CONR6 (wherein R6 = H, alkyl); Z1 = bond, O, S, NH; Z2 = H, alkyl, alkylthio, OH, NH2], useful in treating such bone diseases as osteoporosis, are prepd. A soln. of 1.6M BuLi/hexane was added to a soln. of estratriene II (THP = tetrahydro-2-pyranyl) in THF at 0.degree. and stirred at room temp., to the soln. was added I(CH2)3CMe[PO(OCHMe2)2]2, and the soln. was stirred at room temp. and then acidified to pH 1 to give 96% bisphosphonate III. I at 3 mg/kg s.c. per day in mice for 3 wk gave a bone salt concn. of 120.4 .+-. 3.96 mg/cm2, vs. 103.1 .+-. 2.25 mg/cm2 for controls.

MSTR 1A



G1 = 303



G3 = alkylene<(1-6)>

L11 ANSWER 5 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)
G4 = Ak<EC (1-6) C, BD (0-) D (0-) T>
G7 = NH
G16 = OH
DER: and pharmaceutically acceptable salts
MPL: claim 1
NTE: substitution is restricted

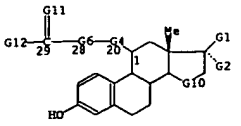
L11 ANSWER 6 OF 7 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 116:214774 MARPAT
TITLE: 19-Norsteroids having an amide-bearing chain in the 11-beta position, their preparation, their use as medicines (especially antiestrogens), and pharmaceutical compositions thereof
INVENTOR(S): Claussner, Andre; Nique, Francois; Teutsch, Jean Georges; Van de Velde, Patrick
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: Eur. Pat. Appl., 63 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 471612	A2	19920219	EP 1991-402214	19910809
EP 471612	A3	19920513		
EP 471612	B1	19980128		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FR 2665901	A2	19920221	FR 1990-10323	19900814
FR 2665901	B2	19940729		
AT 162797	E	19980215	AT 1991-402214	19910809
ES 2112268	T3	19980401	ES 1991-402214	19910809
CA 2049102	AA	19920215	CA 1991-2049102	19910813
HU 59416	A2	19920528	HU 1991-2690	19910813
JP 06340688	A2	19941213	JP 1991-226410	19910813
JP 3073803	B2	20000807		
AU 9182422	A1	19920220	AU 1991-82422	19910814
AU 644671	B2	19931216		
ZA 9106420	A	19921028	ZA 1991-6420	19910814
US 5707982	A	19980113	US 1993-68735	19930528
PRIORITY APPLN. INFO.:			FR 1990-10323	19900814
			FR 1989-2384	19890224
			US 1990-484424	19900223
			US 1991-745289	19910814

AB Twenty title steroids I [either (1) n = 1; K = O; R17 = OH, O2C(CH2)2CO2H or salts; R17' = H, C.tplbond.CH; RA = Me; RB = iso-Pr, Bu, heptafluorobutyl; X = CH2, C6H4, OC6H4; Y = (CH2)7, (CH2)8, (CH2)5C.tplbond.C, (CH2)qOCH2 with q = 5-7, (CH2)5S(O)pCH2 with p = 0-2; Z = bond; or (2) n = 1 or 2; K = O, S; R17 = OH, acyloxy; R17' = H, (substituted) alkyl, alkenyl, or alkynyl; or R17R17' = keto; X = CH2, arylene, OCH2, oxyarylene, thioarylene (bound to steroid at C atom); Y = aliph. chain optionally unsatd. or interrupted by arylene, O, S, SO, or SO2; Z = bond; RA, RB = H, (substituted) alkyl; or RARB = atoms to form (substituted) heterocycle; addnl. restrictions] were prepd. as antiestrogens for treatment of hormone-dependent tumors. For example, 11.beta.-(4-hydroxyphenyl)estra-4,9-diene-3,17-dione was etherified with BuNMeCOCH2O(CH2)5Br (prepns. given), followed by isomerization to a 3-hydroxyestra-1,3,5(10)-triene, redn. of the 17-oxo group to 17.beta.-OH with NaBH4, protection of the OH groups as acetates, conversion of the amide to a thioamide with Lawesson's reagent, and deprotection, to give title compd. II. The IC50 of II for inhibiting growth of MCF-7 mammary tumor cells in vitro was 0.03 nM. A tablet formulation comprising I is given.

MSTR 1B

L11 ANSWER 6 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G1 = OH
G4 = CH2
G6 = Ak<(1-18)>
G10 = (1-2) CH2
G12 = 52

G13 = alkyl<(1-8)> (SO G14)
DER: or salts
MPL: claim 1
NTE: substitution is restricted

L11 ANSWER 7 OF 7 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 115:214857 MARPAT
TITLE: Injectable microspheres containing antiestrogenic and antiprogestomimetic steroids
INVENTOR(S): Cohen, Gerard; Dubois, Jean Luc
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

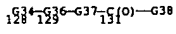
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4036425	A1	19910516	DE 1990-4036425	19901115
FR 2654337	A1	19910517	FR 1989-14976	19891115
FR 2654337	B1	19940805		
SE 9003570	A	19910516	SE 1990-3570	19901109
BE 1005511	A4	19930831	BE 1990-1062	19901109
DK 9002709	A	19910516	DK 1990-2709	19901113
CA 2029940	AA	19910516	CA 1990-2029940	19901114
JP 03294229	A2	19911225	JP 1990-306374	19901114
CH 681691	A	19930514	CH 1990-3611	19901114
NL 9002492	A	19910603	NL 1990-2492	19901115
GB 2239798	A1	19910717	GB 1990-24862	19901115
GB 2239798	B2	19931027		
AT 9002313	A	19950415	AT 1990-2313	19901115
AT 400298	B	19951127		

PRIORITY APPLN. INFO.: FR 1989-14976 19891115

AB Biodegradable microspheres comprise the title steroids (Markush given) and copolymers of lactic acid with glycolic acid. A mixt. of 250 mL aq. 0.3% hydrolyzed PVA soln., 1 g poly(DL-lactic acid-glycolic acid), 17 g CH2Cl2, and 0.5 g 17.beta.-hydroxy-11.beta.-[4-(dimethylamino)phenyl]-17.alpha.-(1-propynyl)estra-4,9-dien-3-one was emulsified, followed by stirring at 22.degree. and decreasing pressure (.gtoreq.400 mm Hg) to give microspheres, which were used for the prepn. of injections.

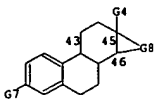
MSTR 18

G1 = 128



G3 = 43

L11 ANSWER 7 OF 7 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G7 = OH
G8 = 88-45 90-46

G18 = OH
G34 = CH2
G38 = alkylamino<(1-8)> (SO (1-) G39)
MPL: claim 6
NTE: Ak<(1-18)> in G36 may be interrupted by an arylene group or an oxygen atom

```
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L1              STRUCTURE UPLOADED
L2            1 S L1
L3           36 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 11:15:38 ON 03 SEP 2003
L4            2 S L3

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L5              STRUCTURE UPLOADED
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L7           47 S L5 FULL

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L8            4 S L7

     FILE 'BEILSTEIN' ENTERED AT 11:21:49 ON 03 SEP 2003
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     FILE 'MARPAT' ENTERED AT 11:24:19 ON 03 SEP 2003
L10           1 S L7
L11           7 S L7 FULL
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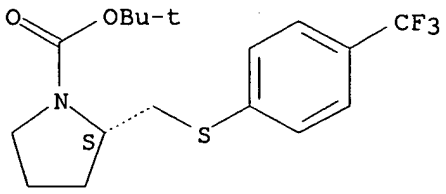
=> d scan

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1-Pyrrolidinecarboxylic acid, 2-[[[4-(trifluoromethyl)phenyl]thio]methyl]-, 1,1-dimethylethyl ester, (2S)- (9CI)
MF **C17 H22 F3 N O2 S**

Absolute stereochemistry.

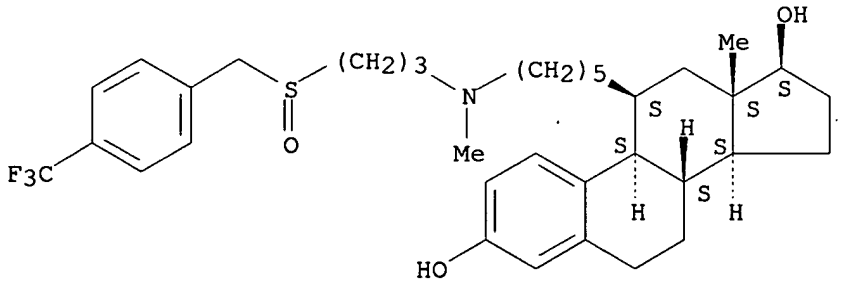


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[[[4-(trifluoromethyl)phenyl]methyl]sulfinyl]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI)
MF **C35 H48 F3 N O3 S**

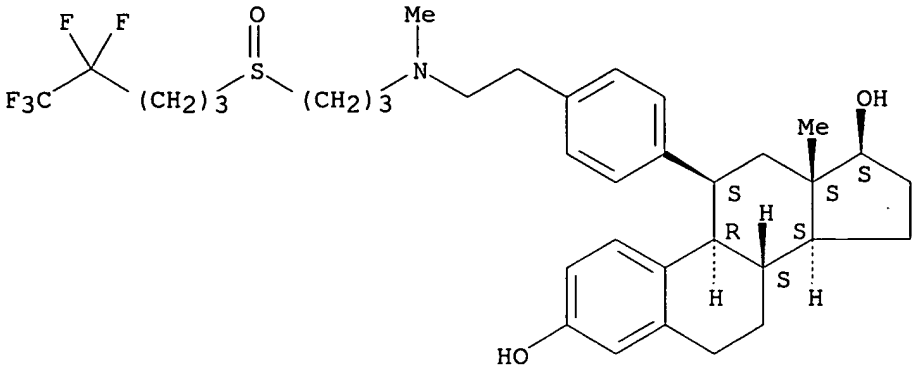
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

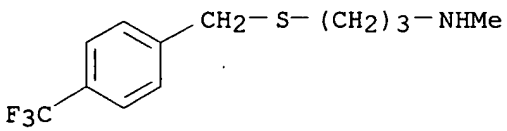
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[4-[2-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]propyl]amino]ethyl]phenyl]-, (11.beta.,17.beta.)- (9CI)
MF **C35 H46 F5 N O3 S**

Absolute stereochemistry.



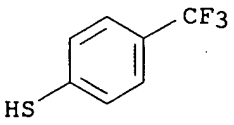
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1-Propanamine, N-methyl-3-[[[4-(trifluoromethyl)phenyl]methyl]thio]- (9CI)
MF **C12 H16 F3 N S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

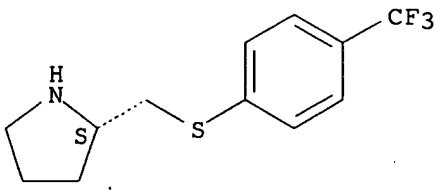
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Benzenethiol, 4-(trifluoromethyl)- (9CI)
MF **C7 H5 F3 S**
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pyrrolidine, 2-[[[4-(trifluoromethyl)phenyl]thio]methyl]-, (2S)- (9CI)
MF **C12 H14 F3 N S**

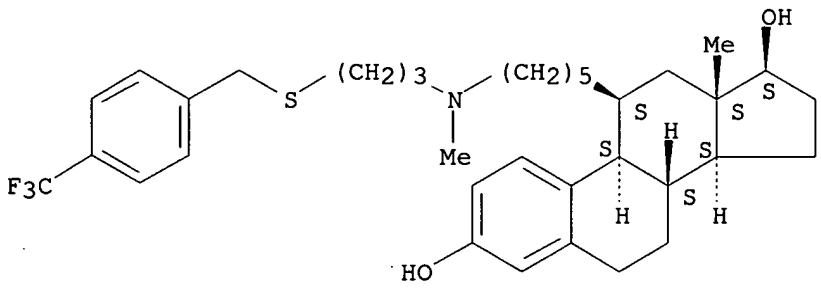
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[[[4-(trifluoromethyl)phenyl]methyl]thio]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI)
MF **C35 H48 F3 N O2 S**

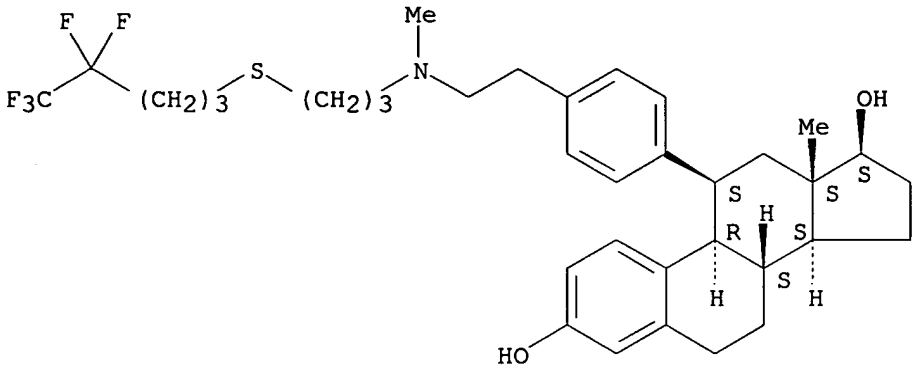
Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

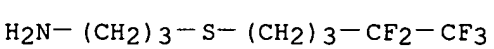
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[4-[2-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]ethyl]phenyl]-, (11.beta.,17.beta.)- (9CI)
MF **C35 H46 F5 N O2 S**

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

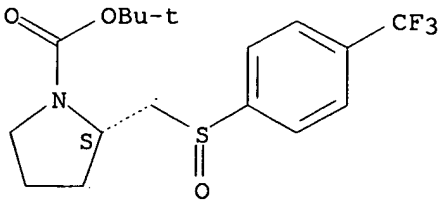
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1-Propanamine, 3-[(4,4,5,5,5-pentafluoropentyl)thio]- (9CI)
MF **C8 H14 F5 N S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

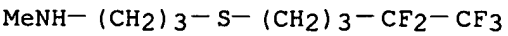
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1-Pyrrolidinecarboxylic acid, 2-[[[4-(trifluoromethyl)phenyl]sulfinyl]methyl]-, 1,1-dimethylethyl ester, (2S)- (9CI)
MF **C17 H22 F3 N O3 S**

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

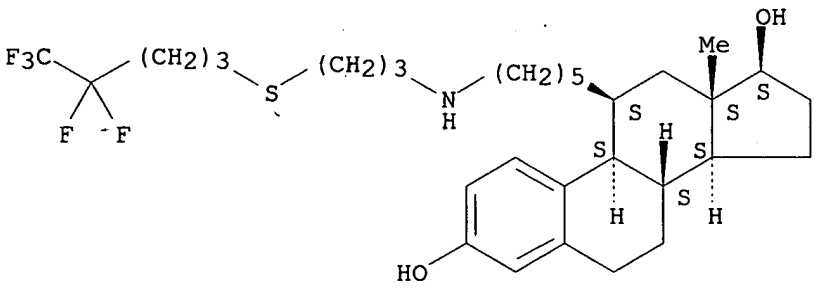
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN 1-Propanamine, N-methyl-3-[(4,4,5,5,5-pentafluoropentyl)thio]- (9CI)
MF **C9 H16 F5 N S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI)
MF **C31 H46 F5 N O2 S**

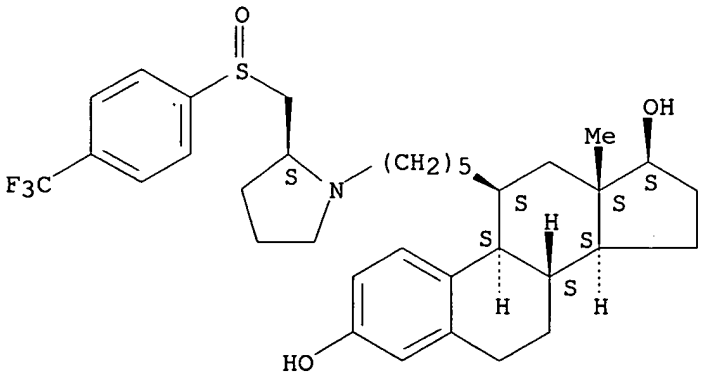
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(2S)-2-[[[4-(trifluoromethyl)phenyl]sulfinyl]methyl]-1-pyrrolidinyl]pentyl]-, (11.beta.,17.beta.)- (9CI)
MF **C35 H46 F3 N O3 S**

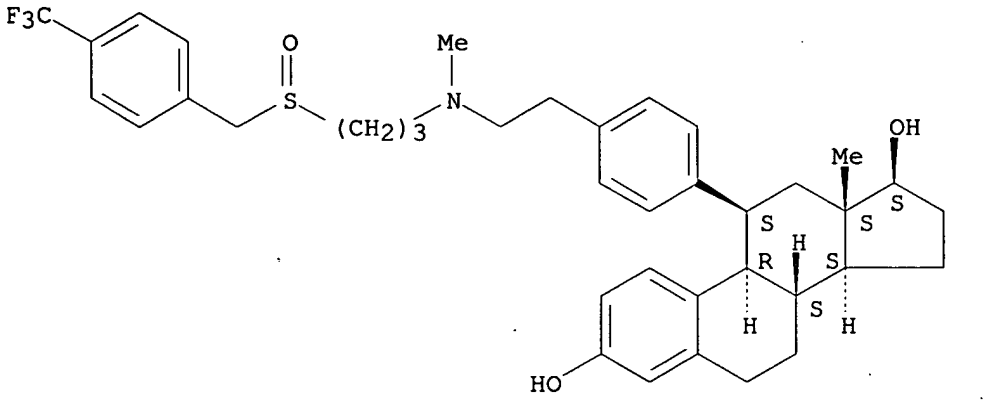
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[4-[2-[methyl[3-[[[4-(trifluoromethyl)phenyl]methyl]sulfinyl]propyl]amino]ethyl]phenyl]-, (11.beta.,17.beta.)- (9CI)
MF **C38 H46 F3 N O3 S**

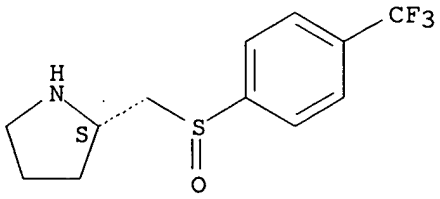
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Pyrrolidine, 2-[[[4-(trifluoromethyl)phenyl]sulfinyl]methyl]-, (2S)- (9CI)
MF **C12 H14 F3 N O S**

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

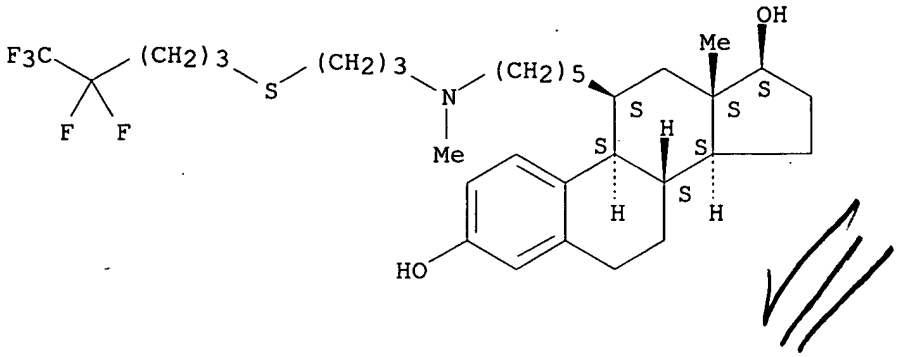
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Ethanethioic acid, S-(4,4,5,5,5-pentafluoropentyl) ester (9CI)
MF **C7 H9 F5 O S**

AcS— $(CH_2)_3$— CF_2— CF_3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[methyl[3-[(4,4,5,5,5-pentafluoropentyl)thio]propyl]amino]pentyl]-, (11.beta.,17.beta.)- (9CI)
MF **C32 H48 F5 N O2 S**

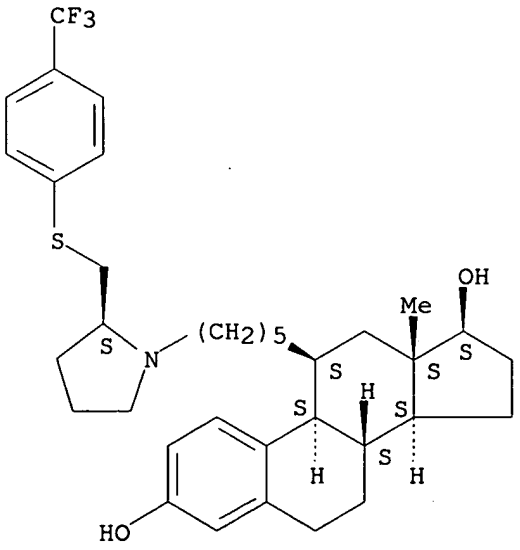
Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[5-[(2S)-2-[[[4-(trifluoromethyl)phenyl]thio]methyl]-1-pyrrolidinyl]pentyl]-, (11.beta.,17.beta.)- (9CI)
MF **C35 H46 F3 N O2 S**

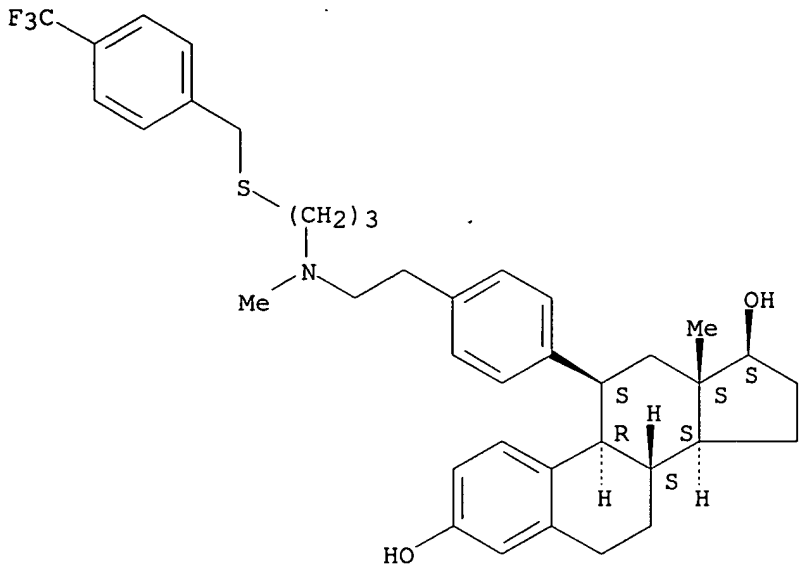
Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

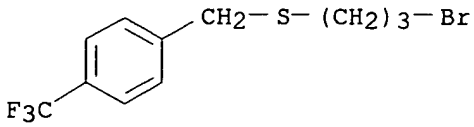
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[4-[2-[methyl[3-[[[4-(trifluoromethyl)phenyl]methyl]thio]propyl]amino]ethyl]phenyl]-, (11.beta.,17.beta.)- (9CI)
MF **C38 H46 F3 N O2 S**

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

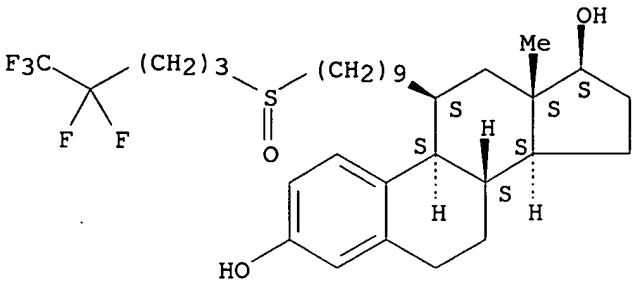
L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Benzene, 1-[[(3-bromopropyl)thio]methyl]-4-(trifluoromethyl)- (9CI)
MF **C11 H12 Br F3 S**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 21 ANSWERS REGISTRY COPYRIGHT 2003 ACS on STN
IN Estra-1,3,5(10)-triene-3,17-diol, 11-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (11.beta.,17.beta.)- (9CI)
MF **C32 H47 F5 O3 S**

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT